

Contents lists available at [SciVerse ScienceDirect](http://SciVerse.ScienceDirect.com)

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

A shell theory with scale effects and higher order gradients

C. Sansour^{a,*,1}, S. Skatulla^b, M. Hjiaj^c^a INSA de Rennes, Department of Civil Engineering, 20 Avenue des Buttes des Cosmes, 25043 Rennes Cedex, France^b CERECAM, Department of Civil Engineering, University of Cape Town, Private Bag X3, Rondebosch 7701, South Africa^c Structural Engineering Research Group/LGCGM, INSA de Rennes, 20 Avenue des Buttes de Cosmes, 35043 Rennes Cedex, France

ARTICLE INFO

Article history:

Received 22 November 2012

Received in revised form 6 February 2013

Available online 15 April 2013

Keywords:

Shell theory

Scale effects

Generalised continua

Strain gradient theory

ABSTRACT

This work follows a generalised continuum framework developed by Sansour (1998) to derive a strain gradient formulation suitable to address scale effects of structures where one dimension is very small (e.g. thin films, nano tubes etc.). Whereas a previous strain gradient approach by Sansour et al. (2009) considered the fully three-dimensional setting, the approach here proposes a shell theory which aims to run computations of thin structures more efficiently and to include scale effects. The theory features a generalised deformation description, new strain and stress measures. As consequence of these new quantities a corresponding generalised variational principle is formulated. The approach is completed by Dirichlet boundary conditions for the displacement field and its derivatives. A numerical example is presented based on a meshfree formulation which provides the necessary C^1 continuity.

Crown Copyright © 2013 Published by Elsevier Ltd. All rights reserved.

1. Introduction

In the classical fields of its applications, non-linear shell theory has achieved a high level of sophistication. Computations of large deformations, also at large strains, elastic or inelastic, can well be performed for shells. In recent times, however, scale effects have come in the research focus due to the fact that they originate in and characterise the material behaviour at lower scales. The latter is considered an important area of research in material science and engineering. Indeed, in many applications scale effects can be observed and 3-dimensional extended theories of deformation have been constructed to cater for them. The lack of scale effects, however, is one of the major shortcomings of classical shell theories. New areas of applications such as in the fields of bio-mechanics and micro-mechanics, where scale effects do play an important role, motivate new approaches to shell theory. The paper is about constructing a geometrically exact shell theory which exhibits scale effects in a natural way and so can capture the same in computations.

Classically, there has been two approaches to derive shell theories. In the first one, the three-dimensional field equations are approximated depending on certain assumptions regarding the displacement field as a function of the shell thickness. The corresponding integration over the shell thickness of the principal

of virtual work, or any equivalent or similar statement such as Hamilton's principle in the dynamical case, leads to reduced two-dimensional field equations. Alternatively, in the so-called direct approach shell theories are derived by considering two-dimensional surfaces from the outset, where these surfaces are equipped with extra degrees of freedom via a generalised-continuum framework. One of the early attempts to do so is the work by Ericksen et al. (1957) which initiated further work half century ago (e.g. Cohen et al., 1966; Green et al., 1965).

In addition to the approach itself, shell theories can be classified depending on the kinematic assumptions underlying their derivation. Of the many possible assumptions two groups are of special interest. In the first group one distinguishes between theories which allow for shear strain to be considered (shearable shells) in contrast to those which assume shear rigidity (Kirchhoff–Love assumption). In the second, the classification follows the consideration whether thickness change is taken into account in contrast to theories which assume the thickness to be constant. The latter classification is of interest with regard to non-linear constitutive laws. Taking shell thickness changes into account allows for those to be applied directly and the reduction to a plane state of stress becomes obsolete. In general, these assumptions decide about the number of degrees of freedom retained in the theory. However, some assumptions can be relaxed within a numerical procedure without increasing the degrees of freedom per se, e.g. thickness change can be introduced via an assumed strain methodology within the numerical scheme.

Shell theories can be classified further regarding the type of strain measures used. Specifically two types can be distinguished: shell theories based on the symmetric Green strain tensor and a

* Corresponding author. Tel.: +44 115 9513874; fax: +44 115 9513898.

E-mail addresses: carlo.sansour@nottingham.ac.uk (C. Sansour), sebastian.skatulla@uct.ac.za (S. Skatulla), Mohammed.Hjiaj@insa-rennes.fr (M. Hjiaj).¹ On leave from Department of Civil Engineering, The University of Nottingham, University Park, Nottingham NG7 2RD, United Kingdom.

corresponding symmetric change of curvature tensor (metric-based strain measures), and those based on stretch type strain measures, symmetric or otherwise, together with corresponding change of curvature tensor.

Examples of Kirchhoff–Love type shells can be found in Koiter (1963); Pietraszkiewicz (1974) Pietraszkiewicz (1989); Schieck et al. (1992); Cirak et al. (2000). Shearable shells with so-called Reissner–Mindlin kinematics were formulated by Naghdi (1972) and parameterised by a 2-dimensional rotation tensor by Simo et al. (1990), see also Basar et al. (1990), Bischoff et al. (1997), Klinkel et al. (2008). Stretch-type strain measures in conjunction with a three-parametric rotation tensor, formulated with shear but with no thickness change, can be found in E. Reissner (1983); Libai et al., 1983 and Zhilin (1976), all in intrinsic formulations, and in Sansour et al. (1992); Sansour et al. (1995); Chrosielewski et al. (1992); Merlini et al. (2011) with explicit inclusion of rotation tensors. Shells with thickness change have been formulated in Sansour et al. (1995); Parisch (1995); and Sansour et al. (1998) via corresponding degrees of freedom and in Buechter et al. (1994) via an assumed strain ansatz.

Within finite element frameworks non-linear shells which fall in one of the above categories or modification thereof have been widely considered in the literature. The list would be too long to call, however, among many others we mention Wriggers et al. (1993); Betsch et al. (1996); Ibrahimbegovic et al. (1235); Kulikov et al. (2002); Arciniega et al. (2007); Reias et al. (2005); Dung et al. (2008).

To derive a shell theory with scale effects, the area of generalised continua is a natural starting point. In contrast to classical continuum theories, generalised formulations facilitate internal lengths which can describe scale effects (Eringen, 1999). The incorporation of strain gradients were shown to be useful in avoiding difficulties associated with strain and stress singularities (see e.g. Lazar et al., 2006), or provide scale effects (Aifantis, 1999; Akarapu et al., 2006; Ohashi et al., 1307). For the former, material instabilities linked with the loss of ellipticity of the governing equations can be dealt with, e.g. as observed in shear band formations. Generalised continua also found application in higher-order homogenisation schemes incorporating strain gradients and micro-space boundary conditions (Kouznetsova et al., 1235; Larsson et al., 2006). A few recent applications of generalised continuum formulations, though linear ones, are reported in Manzarria et al. (2005); Kumar et al. (2004); Dillard et al. (2006).

Many applications, however, are concerned with so-called thin domains (e.g. thin films, nano tubes). These kinds of computations can be more effectively run via a shell theory. Hence the motivation to develop a shell theory which includes in a natural way scale effects. This is done by extending and modifying existing 3D generalised formulations of the authors (Sansour, 1998; Sansour et al., 2009) to accommodate for the shell. A rather simplified strain gradient theory was employed in Sun et al. (2008) and implemented in a meshfree code to study higher order effects modelling the buckling behaviour of nanotubes under torsion and axial compression, respectively. In Papargyri-Beskou (2009) a formulation for special cylindrical shells under axial compressive forces with simplified Donnell-type non-linearity was considered and in Reddy (2010) a non-local plate theory with simple von Karman-type non-linearity was presented.

This generalised continuum framework considers a generalised space consisting of a macro- and micro-continuum. The generalised position vector is consequently a function of corresponding macro and micro co-ordinates. However, the dependency on the micro co-ordinates is assumed to be a priori known. For specific choices, specific generalised continuum theories are recovered. The dimensionality of the micro-continuum and the number of degrees of freedom additional to those needed for a classical

continuum or equivalently, the use of higher order deformations, may be freely chosen depending on the accuracy desired in the description of the physical process at hand. In particular, for fully non-linear formulations including inelastic deformations at finite strains, the strength and generality of the formulation can be completely exploited. Most notably, the difference in the number of material parameters in comparison to a classical formulation is kept to a minimum and is confined to purely geometric ones which describe the micro continuum. In this paper, the approach is modified as to account for two different internal or micro spaces. The first one is supposed to capture the thickness effects and the second captures the scale effects. The approach provides strain measures which go beyond the membrane strain and the change of curvature tensor, the classical strain measures of the shell. The resulting theory takes shear and thickness change into account but considers also higher gradient responsible for the scale effects.

The paper is organised as follows: In Section 2 the theory of the three-dimensional generalised continuum is outlined and then modified in Section 3 to specifically address shell structures exhibiting scale effects. Subsequently, in Section 4 a variational formulation based on the generalised shell theory is proposed. A numerical example utilizing hyperelastic material law and moving least square (MLS)-based approximations is presented in Section 6.

2. Deformation and strain

The generalised continuum theory which will be outlined in the following is based on the theoretical framework for a generalised continuum proposed in Sansour (1998). This framework makes use of the mathematical concept of a fibre bundle, where, in the simplest case, the generalised space is constructed as the Cartesian product of a macro space $\mathcal{B} \subset \mathbb{E}(3)$ and a micro-space \mathcal{S} which we write as $\mathcal{G} := \mathcal{B} \times \mathcal{S}$. This definition assumes an additive structure of \mathcal{G} which implies that the integration over the macro- and the micro-continuum can be performed separately. Physically, the micro-continuum can be related to what is known as the representative volume element. However, the concept here is very general in nature as it allows for such a continuum to be of any dimension, also one-dimensional. The macro-space \mathcal{B} is parameterized by the curvilinear coordinates ϑ^i and the micro-space \mathcal{S} by the curvilinear coordinates ζ^α , both we assume to be convected. Here, and in what follows, Latin indices take the values 1, 2 or 3 and Greek indices 1, ... or n . The dimension of \mathcal{S} denoted by n is arbitrary, but finite. Furthermore, we want to exclude that the dimension and topology of the micro-space is dependent on ϑ^i .

Each material point $\tilde{\mathbf{X}} \in \mathcal{G}$ is related to its spatial placement $\tilde{\mathbf{x}} \in \mathcal{G}_t$ at time $t \in \mathbb{R}$ by the mapping $\tilde{\varphi}(t) : \mathcal{G} \rightarrow \mathcal{G}_t$ as illustrated in Fig. 1. Note the generalised space \mathcal{G} is indicated by a swung dash and for convenience, but without loss of generality, we identify \mathcal{G} with the un-deformed reference configuration at a fixed time t_0 , here and in what follows.

The generalised space can be projected to the macro-space in its reference and its current configuration by

$$\pi_0(\tilde{\mathbf{X}}) = \mathbf{X} \quad \text{and} \quad \pi_t(\tilde{\mathbf{x}}) = \mathbf{x} \quad (1)$$

respectively, where π_0 as well as π_t represent projection maps, and $\mathbf{X} \in \mathcal{B}$ and $\mathbf{x} \in \mathcal{B}_t$. The tangent space $\mathcal{T}\mathcal{G}$ in the reference configuration and $\mathcal{T}\mathcal{G}_t$ at the current configuration are given by the pairs $(\tilde{\mathbf{G}}_i \times \mathbf{I}_\alpha)$ and $(\tilde{\mathbf{g}}_i \times \mathbf{i}_\alpha)$, respectively, which are defined by

$$\tilde{\mathbf{G}}_i = \frac{\partial \tilde{\mathbf{X}}}{\partial \vartheta^i} \quad \text{and} \quad \mathbf{I}_\alpha = \frac{\partial \tilde{\mathbf{X}}}{\partial \zeta^\alpha}, \quad \tilde{\mathbf{g}}_i = \frac{\partial \tilde{\mathbf{x}}}{\partial \vartheta^i} \quad \text{and} \quad \mathbf{i}_\alpha = \frac{\partial \tilde{\mathbf{x}}}{\partial \zeta^\alpha}. \quad (2)$$

The corresponding dual contra-variant vectors are denoted by $\tilde{\mathbf{G}}^i$ and \mathbf{I}^α , respectively. The generalised tangent space can also be projected to its corresponding macro-space by

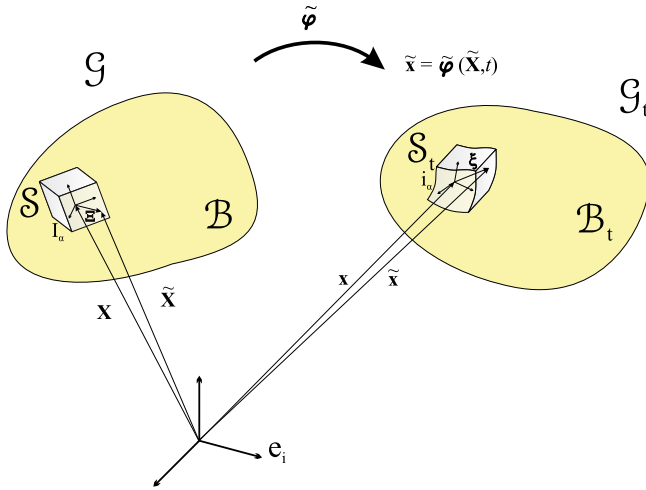


Fig. 1. configuration spaces.

$$\pi_0^*(\tilde{\mathbf{G}}_i) = \mathbf{G}_i \quad \text{and} \quad \pi_t^*(\tilde{\mathbf{g}}_i) = \mathbf{g}_i \quad (3)$$

respectively. Note that the idea of a projection is not trivial. The definition of the projection maps depends on the geometry and the topology of the micro-space. While it is possible to assume a Cartesian micro-space, resulting in a projection map which is the identity, in general, however, the micro-space could be equipped with a curvature or has a complicated topological structure resulting in non-trivial projection maps

Now, we assume that the placement vector $\tilde{\mathbf{x}}$ of a material point P ($\tilde{\mathbf{X}} \in \mathcal{G}$) is of an additive nature and is the sum of its position in the macro-continuum $\mathbf{x} \in \mathcal{B}_t$ and in the micro-continuum $\xi \in \mathcal{S}_t$ as follows

$$\tilde{\mathbf{x}}(\vartheta^k, \zeta^\alpha, t) = \mathbf{x}(\vartheta^k, t) + \xi(\vartheta^k, \zeta^\alpha, t). \quad (4)$$

Thereby, the micro-placement ξ is taken relative to the macro-placement vector \mathbf{x} .

Remark. It is important to note that while we view the deformation in a higher dimensional space, the final goal is to project this deformation on the classical three dimensional space (that is on \mathcal{B}). When doing so we end up with a richer type of deformations, extra degrees of freedom and a scheme as to how to determine the constitutive law for them. Now, in the deformed configuration, Eq. (4), $\tilde{\mathbf{x}}$ has components in all dimensions of the extended space and so does ξ . \mathbf{x} is by definition the projection on \mathcal{B}_t . However, since we are interested in the projections, that is, in what happens in the classical three-dimensional space, we can restrict ourselves to these vectors being defined in \mathbb{R}^3 , specifically to the components of ξ in that space. This can be done either by restricting the map $\tilde{\varphi}$ to \mathbb{R}^3 or by considering only the projection of $\tilde{\varphi}$ on that space. Of course it is possible to run the computations in the whole extended space but, unless there is a necessity to do so, it is much more economical and practical to restrict the vectors to three dimensions.

At the heart of the approach is the assumption that the dependency of ξ on the co-ordinate ζ^α can be given a priori in form of an ansatz. The assumption $\zeta^\alpha/R \ll 1$, justifies the simplest possible choice of linear dependency which leads to the following ansatz:

$$\tilde{\mathbf{x}} = \mathbf{x}(\vartheta^k, t) + \zeta^\alpha \mathbf{a}_\alpha(\vartheta^k, t). \quad (5)$$

The vectors $\mathbf{a}_\alpha(\vartheta^k, t)$ can be viewed as the extra degrees of freedom of the system with their corresponding micro-coordinates ζ^α and

their direction coinciding with \mathbf{i}_α as depicted in Fig. 1. The number of these vectors must be chosen according to a specific topology of the micro-space as well as certain physical properties of a material due to its intrinsic structure. Generally, the vector functions $\mathbf{a}_\alpha(\vartheta^k, t)$ can be described with the help of a tensor \mathbf{A} as follows

$$\mathbf{a}_\alpha(\vartheta^k, t) = \mathbf{A} \mathbf{i}_\alpha. \quad (6)$$

Note, if the dimension of \mathcal{S} is three, then we have $\mathbf{A} \in GL^+(3)$ which can be restricted to subgroups of $GL^+(3)$ as well. Here $GL^+(3, \mathbb{R})$ defines the general linear group of 3×3 matrices (defined over the body of real numbers) with positive determinants (simply all invertible 3×3 matrices with positive determinants).

In order to avoid the incorporation of additional degrees of freedom, other than the displacement degrees of freedom, we first restrict the dimensionality of the micro-space to three; Greek indices take now the values 1, 2, or 3. Second, we define the extra degrees of freedom \mathbf{a}_α (Eq. 6) in the current configuration \mathcal{B}_t from now on as follows

$$\mathbf{a}_\alpha = \frac{\partial \mathbf{x}}{\partial \vartheta^1}, \quad \frac{\partial \mathbf{x}}{\partial \vartheta^2}, \quad \text{or} \quad \frac{\partial \mathbf{x}}{\partial \vartheta^3}. \quad (7)$$

Note, that it is important to realize that the dimension of the micro-space does not have to coincide with the dimension of the macro-space, but must not be larger than three.

Taking the spatial derivatives of the position vector in the current configuration with respect to the macro-coordinates ϑ^i given by

$$\tilde{\mathbf{x}}_{,i} = \frac{\partial \tilde{\mathbf{x}}}{\partial \vartheta^i} = \mathbf{x}_{,i}(\vartheta^k, t) + \zeta^\alpha \mathbf{a}_{\alpha,i}(\vartheta^k, t) \quad (8)$$

and with respect to the micro-coordinates ζ^α given by

$$\tilde{\mathbf{x}}_{,\alpha} = \frac{\partial \tilde{\mathbf{x}}}{\partial \zeta^\alpha} = \mathbf{a}_\alpha(\vartheta^k, t), \quad (9)$$

the generalised deformation gradient tensor is then expressed as follows

$$\tilde{\mathbf{F}} = (\mathbf{x}_{,i} + \zeta^\alpha \mathbf{a}_{\alpha,i}) \otimes \tilde{\mathbf{G}}^i + \mathbf{a}_{\alpha} \otimes \mathbf{I}^\alpha. \quad (10)$$

Note that second order derivatives now have entered the formulation. This is a direct consequence of restricting the degrees of freedom to those of a classical continuum, while still keeping to a generalised deformation.

In order to formulate generalised strain measures we proceed in analogy to the definition of the classical right Cauchy–Green deformation tensor and define its generalised equivalent as

$$\tilde{\mathbf{C}} = \tilde{\mathbf{F}}^T \tilde{\mathbf{F}}. \quad (11)$$

By neglecting higher order terms in ζ^α as well as restricting ourselves, for the sake of mathematical simplicity and computational performance, to the physically meaningful projections on $\mathbb{R}^3 \times \mathbb{R}^3$, by disregarding contributions with respect to $\tilde{\mathbf{G}}^k \otimes \mathbf{I}^\beta$ and $\mathbf{I}^\alpha \otimes \mathbf{I}^\beta$, we get

$$\tilde{\mathbf{C}} = (\mathbf{x}_{,k} \cdot \mathbf{x}_{,l} + \zeta^\alpha (\mathbf{x}_{,k} \cdot \mathbf{a}_{\alpha,l} + \mathbf{a}_{\alpha,k} \cdot \mathbf{x}_{,l})) \tilde{\mathbf{G}}^k \otimes \tilde{\mathbf{G}}^l = \mathbf{C} + \zeta^\alpha \mathbf{K}_\alpha. \quad (12)$$

This is a meaningful outcome, because $\tilde{\mathbf{C}}$ still includes the conventional as well as the generalised type of strains. \mathbf{C} represents the conventional right Cauchy–Green deformation tensor and \mathbf{K}_α the generalised contributions of Eq. (12). Note that the scalar products of vectors are denoted by a dot.

3. generalised shell theory

To derive a shell theory with scale effects the above framework is modified and extended in two ways. First, the generalised space

is assumed to consist of two fibres the product of which is defined as follows:

$$\mathcal{G} := \{\mathcal{B} \times \mathcal{L}\} \times \mathcal{S}. \quad (13)$$

Here, \mathcal{L} is a further fibre the geometric nature of which is to be specified depending on the problem at hand. Second, with shell theory in mind, the above space is specified by certain selection of the dimensions of \mathcal{B} and \mathcal{L} . Specifically \mathcal{B} is assumed to be a two-dimensional continuum, henceforth referred to as \mathcal{M} , and \mathcal{L} is assumed to be a one-dimensional continuum. Accordingly, we have

$$\mathcal{G} := \{\mathcal{M} \times \mathcal{L}\} \times \mathcal{S}. \quad (14)$$

\mathcal{M} is supposed to model a two-dimensional surface parameterised by the curvilinear coordinates ϑ^i and \mathcal{L} is supposed to model the shell thickness which is parameterised by the generally curvilinear coordinate z . The microspace \mathcal{S} is again parameterised by the curvilinear co-ordinates ζ^α . Accordingly, in what follows, Latin indices take the values 1 or 2, and Greek indices 1, ..., to n .

The tangent space $\mathcal{T}\mathcal{G}$ in the reference configuration is defined now by the triple $\{(\tilde{\mathbf{G}}_i \times \tilde{\mathbf{N}}) \times \tilde{\mathbf{I}}_z\}$ given by

$$\tilde{\mathbf{G}}_i = \frac{\partial \tilde{\mathbf{X}}}{\partial \vartheta^i}, \quad \tilde{\mathbf{N}} = \frac{\partial \tilde{\mathbf{X}}}{\partial z} \quad \text{and} \quad \tilde{\mathbf{I}}_z = \frac{\partial \tilde{\mathbf{X}}}{\partial \zeta^\alpha}. \quad (15)$$

The corresponding tangent space in the current configuration $\mathcal{T}\mathcal{G}_t$ is spanned by the triple $\{(\tilde{\mathbf{g}}_i \times \tilde{\mathbf{d}}) \times \tilde{\mathbf{i}}_z\}$ given by

$$\tilde{\mathbf{g}}_i = \frac{\partial \tilde{\mathbf{x}}}{\partial \vartheta^i}, \quad \tilde{\mathbf{d}} = \frac{\partial \tilde{\mathbf{x}}}{\partial z} \quad \text{and} \quad \tilde{\mathbf{i}}_z = \frac{\partial \tilde{\mathbf{x}}}{\partial \zeta^\alpha}. \quad (16)$$

At the shell surface the pair $(\mathbf{G}_i, \mathbf{N})$ defines the natural covariant base of the macro-space (or base continuum) $\mathcal{M} \times \mathcal{L}$ in the reference configuration, whereas \mathbf{g}_i and \mathbf{d} denote their images in the current configuration. It is convenient to choose \mathbf{N} , via a suitable parametrisation, as the unit normal vector on \mathcal{M} : $\mathbf{N} = \epsilon^{ij} \mathbf{G}_i \times \mathbf{G}_j$, where ϵ^{ij} denotes the components of the two-dimensional Ricci tensor given by

$$\epsilon^{ij} = \begin{cases} +\frac{1}{\sqrt{G}}, & \text{for even permutations of } i, j \\ -\frac{1}{\sqrt{G}}, & \text{for odd permutations of } i, j \end{cases} \quad (17)$$

with \mathbf{G}_i denoting the tangent vectors at \mathcal{M} which are given by $\partial \mathbf{X} / \partial \vartheta^i = \mathbf{G}_i|_{z=0, \zeta=0}$ and G is the determinant of the Riemannian metric coefficients $G_{ij} = \mathbf{G}_i \cdot \mathbf{G}_j$. Note, however, that the vector $\tilde{\mathbf{d}}$, in general, is neither normal to the deformed surface \mathcal{M}_t nor is a unit vector. Such restrictions could be considered which would identify the shell theory as of the Kirchhoff–Love type.

The generalised space is to be projected onto the macro-spaces in their reference and current configurations. Two types of projection maps can be identified. The first onto $(\mathcal{M} \times \mathcal{L})$ and the second one onto \mathcal{M} :

$$\pi_0^{\mathcal{L}}(\tilde{\mathbf{X}}) = \mathbf{X} + \mathbf{Z} \quad \text{and} \quad \pi^{\mathcal{L}}(\tilde{\mathbf{x}}) = \mathbf{x} + \mathbf{z}, \quad (18)$$

as well as

$$\pi_0^{\mathcal{M}}(\tilde{\mathbf{X}}) = \mathbf{X} \quad \text{and} \quad \pi^{\mathcal{M}}(\tilde{\mathbf{x}}) = \mathbf{x}, \quad (19)$$

respectively, where $\mathbf{X} \in \mathcal{M}$, $\mathbf{Z} \in \mathcal{L}$, $\mathbf{x} \in \mathcal{M}_t$ and $\mathbf{z} \in \mathcal{L}_t$. The exact definition of these projections depends on the geometry of the shell, i.e. its curvature, as well as the assumed geometry of the extra space \mathcal{S} . Clearly, while $\pi_0^{\mathcal{M}}, \pi_0^{\mathcal{L}}$ are to be given a priori, their time dependent counterparts will depend on the deformation itself.

The generalised tangent space can also be projected onto its corresponding macro tangent spaces by the corresponding projections

$$\pi_0^{\mathcal{L}*}(\tilde{\mathbf{G}}_i) = \tilde{\mathbf{G}}_i|_{\zeta^\alpha=0}, \quad \pi_0^{\mathcal{L}*}(\tilde{\mathbf{N}}) = \tilde{\mathbf{N}}|_{\zeta^\alpha=0} \quad (20)$$

and

$$\pi_t^{\mathcal{L}*}(\tilde{\mathbf{g}}_i) = \tilde{\mathbf{g}}_i|_{\zeta^\alpha=0}, \quad \pi_t^{\mathcal{L}*}(\tilde{\mathbf{d}}) = \tilde{\mathbf{d}}|_{\zeta^\alpha=0}, \quad (21)$$

as well as

$$\pi_0^{\mathcal{M}*}(\tilde{\mathbf{G}}_i) = \mathbf{G}_i, \quad \pi_0^{\mathcal{M}*}(\tilde{\mathbf{N}}) = \mathbf{N} \quad (22)$$

and

$$\pi_t^{\mathcal{M}*}(\tilde{\mathbf{g}}_i) = \mathbf{g}_i, \quad \pi_t^{\mathcal{M}*}(\tilde{\mathbf{d}}) = \mathbf{d}. \quad (23)$$

Specifically, if we assume that $\tilde{\mathbf{G}}_i = \tilde{\mathbf{G}}_i|_{\zeta^\alpha=0}$, that is $\pi_0^{\mathcal{L}*}$ is the identity map, which means that the extra space \mathcal{S} has no curvature, and in addition that the projection $\pi_0^{\mathcal{M}*}$ acts on $\tilde{\mathbf{N}}$ as the identity map as well, meaning: $\tilde{\mathbf{N}} = \mathbf{N}$, then $\pi_0^{\mathcal{M}*}$ becomes the so-called shifter known in shell theory and is given by the relation $(\mathbf{1} - z\mathbf{B})$, where $\mathbf{1}$ is the identity tensor and \mathbf{B} is the shell curvature tensor. Such a choice of geometry provides us with $\mathbf{Z} = z\mathbf{N}$. In what follows we assume that $z/R \ll 1$, where R is the characteristic length of the shell, which could be its smallest radius.

Now, similar to Eq. (4) we choose the placement vector $\tilde{\mathbf{x}}$ of a material point $P \in \mathcal{G}$ to be the sum of its position in the macro-continuum given by $\mathbf{x} \in \mathcal{M}_t$ as well as $\mathbf{z} \in \mathcal{L}_t$ and its position in the micro-continuum $\xi \in \mathcal{S}_t$ as follows

$$\tilde{\mathbf{x}} = \mathbf{x}(\vartheta^k, t) + \mathbf{z}(\vartheta^k, z, t) + \xi(\vartheta^k, z, \zeta^\beta, t). \quad (24)$$

Note here the dependencies on different sets of co-ordinates. Indeed, in addition to the time, while \mathbf{x} depends on the co-ordinates ϑ^k , \mathbf{z} depends on ϑ^k and z as well. Finally, ξ depends on all co-ordinates ϑ^k, z and ζ^β .

The fundamental step now is to assume the form of the dependencies on z and ζ^β via an appropriate ansatz. We formulate this in two steps. First we assume for $\mathbf{z}(\vartheta^k, z, t)$ a quadratic distribution with respect to z . This is meaningful as it allows for the application of classical three-dimensional constitutive laws without ill-conditioning in the very thin regime (Sansour et al., 1995). Accordingly, we have

$$\tilde{\mathbf{x}} = \mathbf{x}(\vartheta^k, t) + (z + z^2 \lambda(\vartheta^k, t)) \mathbf{d}(\vartheta^k, t) + \xi(\vartheta^k, z, \zeta^\beta, t). \quad (25)$$

The quadratic ansatz in Eq. (25) is a special ansatz not a standard one. Only a scalar term is added which results in a full rank change of curvature tensor ($K_{33} \neq 0$, see below). This fact allows for the application of a three-dimensional constitutive law. In a classical shell formulation we end up with a 7-parameter shell model, as introduced in Sansour et al. (1995); Parisch (1995); and Buechter et al. (1994), the latter in a modified form. The ansatz does not aim at improving the quality of a shell solution linear in z but rather to allow for a full three-dimensional constitutive law to be applied. A mathematical analysis of the model for plates is available in Roesle et al. (1999).

The next step is now to select a function in z, ζ^β for $\xi(\vartheta^k, z, \zeta^\beta, t)$. The simplest possible choice is linear in ζ^β and z as well. Hence, two additional terms must be provided resulting in the following expression:

$$\tilde{\mathbf{x}} = \mathbf{x}(\vartheta^k, t) + [z + z^2 \lambda(\vartheta^k, t)] \mathbf{d}(\vartheta^k, t) + \zeta^\alpha [\mathbf{a}_\alpha(\vartheta^k, t) + z \mathbf{b}_\alpha(\vartheta^k, t)]. \quad (26)$$

This assumption characterises the shell theory at hand. It reduces to a classical shell model if the vectors \mathbf{a}_α and \mathbf{b}_α are disregarded. With them we end up with a shell theory with 7 degrees of freedom for the classical part (\mathbf{x}, \mathbf{d} , and λ) and further two vectors the number of the components of which depends on the dimension of the micro space. Already the simplest one-dimensional choice provides us with two vectors, and so, with extra six degrees of freedom. It is, hence, meaningful to think of simplifications to reduce the overall

number of degrees of freedom. This is to happen in Section 5. For now we derive, based on the above assumption, the strain measures of the shell which are to be retained in any possible analysis.

Since we have assumed that both $z/R \ll 1$ and $\zeta^\alpha/R \ll 1$ we may drop the vectors \mathbf{b}_α which come with the nonlinear term $z\zeta^\alpha$. However, with an eye on the modification of the shell theory, to be addressed later, to include higher gradients of the classical degrees of freedom \mathbf{x} and \mathbf{d} , we retain these vectors as they allow for a symmetric (equal) treatment of both mentioned fields.

Taking the spatial derivatives of the generalised placement vector in the current configuration, Eq. (26), with respect to the macro-coordinates ϑ^i and z as well as with respect to the micro-coordinates ζ^α , the generalised deformation gradient can be written down as follows

$$\tilde{\mathbf{F}} = (\mathbf{x}_i + (z + z^2\lambda)\mathbf{d}_i + z^2\lambda_i\mathbf{d} + \zeta^\alpha\mathbf{a}_{\alpha,i} + z\zeta^\alpha\mathbf{b}_{\alpha,i}) \otimes \tilde{\mathbf{G}}^i + ((1 + 2z\lambda)\mathbf{d} + \zeta^\alpha\mathbf{b}_{\alpha,z}) \otimes \tilde{\mathbf{N}} + (\mathbf{a}_\alpha + z\mathbf{b}_\alpha) \otimes \tilde{\mathbf{I}}^\alpha. \quad (27)$$

Similar to Eq. (11) a generalised *Cauchy-Green* deformation tensor can be formulated. In doing so we restrict ourselves to the dominant and relevant terms. We, accordingly, disregard higher order terms in z and ζ^α as well as the components with respect to $\tilde{\mathbf{G}}^k \otimes \tilde{\mathbf{I}}^\beta$, $\tilde{\mathbf{N}} \otimes \tilde{\mathbf{I}}^\beta$ and $\tilde{\mathbf{I}}^\alpha \otimes \tilde{\mathbf{I}}^\beta$. One has

$$\begin{aligned} \tilde{\mathbf{C}} = & [\mathbf{x}_i \cdot \mathbf{x}_j + z(\mathbf{x}_i \cdot \mathbf{d}_j + \mathbf{d}_i \cdot \mathbf{x}_j) + \zeta^\alpha(\mathbf{x}_i \cdot \mathbf{a}_{\alpha,j} + \mathbf{a}_{\alpha,i} \cdot \mathbf{x}_j) \\ & + \zeta^\alpha(\mathbf{x}_i \cdot \mathbf{b}_{\alpha,j} + \mathbf{x}_j \cdot \mathbf{b}_{\alpha,i} + \mathbf{a}_{\alpha,i} \cdot \mathbf{d}_j + \mathbf{a}_{\alpha,j} \cdot \mathbf{d}_i)] \tilde{\mathbf{G}}^i \otimes \tilde{\mathbf{G}}^j \\ & + [\mathbf{x}_i \cdot \mathbf{d} + z(\mathbf{d}_i \cdot \mathbf{d} + 2\lambda\mathbf{x}_i \cdot \mathbf{d}) + \zeta^\alpha(\mathbf{x}_i \cdot \mathbf{b}_\alpha + \mathbf{a}_{\alpha,i} \cdot \mathbf{d}) \\ & + \zeta^\alpha(2\lambda\mathbf{a}_{\alpha,i} \cdot \mathbf{d} + \mathbf{d} \cdot \mathbf{b}_{\alpha,i} + \mathbf{d}_i \cdot \mathbf{b}_\alpha)] (\tilde{\mathbf{G}}^i \otimes \tilde{\mathbf{N}} + \tilde{\mathbf{N}} \otimes \tilde{\mathbf{G}}^i) \\ & [\mathbf{d} \cdot \mathbf{d} + 4z\lambda\mathbf{d} \cdot \mathbf{d} + \zeta^\alpha 2\mathbf{d} \cdot \mathbf{b}_\alpha + 4z\zeta^\alpha\lambda\mathbf{d} \cdot \mathbf{b}_\alpha] (\tilde{\mathbf{N}} \otimes \tilde{\mathbf{N}}). \end{aligned} \quad (28)$$

The above expression suggests the following strain measures to be considered as the main ones characterising the shell theory:

$$\mathbf{C}_0 = \mathbf{x}_i \cdot \mathbf{x}_j (\mathbf{G}^i \otimes \mathbf{G}^j) + \mathbf{x}_i \cdot \mathbf{d} (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) + \mathbf{d} \cdot \mathbf{d} (\mathbf{N} \otimes \mathbf{N}), \quad (29)$$

$$\mathbf{K} = (\mathbf{x}_i \cdot \mathbf{d}_j + \mathbf{d}_i \cdot \mathbf{x}_j) (\mathbf{G}^i \otimes \mathbf{G}^j) + (\mathbf{d}_i \cdot \mathbf{d} + 2\lambda\mathbf{x}_i \cdot \mathbf{d}) (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) + 4\lambda\mathbf{d} \cdot \mathbf{d} (\mathbf{N} \otimes \mathbf{N}), \quad (30)$$

$$\mathbf{D}_\alpha = (\mathbf{x}_i \cdot \mathbf{a}_{\alpha,j} + \mathbf{a}_{\alpha,i} \cdot \mathbf{x}_j) (\mathbf{G}^i \otimes \mathbf{G}^j) + (\mathbf{x}_i \cdot \mathbf{b}_\alpha + \mathbf{a}_{\alpha,i} \cdot \mathbf{d}) (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) + 2\mathbf{d} \cdot \mathbf{b}_\alpha (\mathbf{N} \otimes \mathbf{N}), \quad (31)$$

$$\begin{aligned} \mathbf{H}_\alpha = & (\mathbf{x}_i \cdot \mathbf{b}_{\alpha,j} + \mathbf{x}_j \cdot \mathbf{b}_{\alpha,i} + \mathbf{a}_{\alpha,i} \cdot \mathbf{d}_j + \mathbf{a}_{\alpha,j} \cdot \mathbf{d}_i) (\mathbf{G}^i \otimes \mathbf{G}^j) \\ & + (2\lambda\mathbf{a}_{\alpha,i} \cdot \mathbf{d} + \mathbf{d} \cdot \mathbf{b}_{\alpha,i} + \mathbf{d}_i \cdot \mathbf{b}_\alpha) (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) \\ & + 4\lambda\mathbf{d} \cdot \mathbf{b}_\alpha (\mathbf{N} \otimes \mathbf{N}). \end{aligned} \quad (32)$$

The above strain measures are defined with respect to the basis system of the shell surface. In order to produce the generalised Cauchy-Green tensor defined in Eq. (28) we first introduce the new strain tensor

$$\mathbf{C} = \mathbf{C}_0 + z\mathbf{K} + \zeta^\alpha\mathbf{D}_\alpha + z\zeta^\alpha\mathbf{H}_\alpha, \quad (33)$$

which must then be projected on the generalised space via the inverse of the tangent projection maps. The relation then holds

$$\tilde{\mathbf{C}} = (\pi_0^{M*})^{-1} \mathbf{C} (\pi_0^{M*})^{-T}. \quad (34)$$

Indeed, while \mathbf{C} and \mathbf{K} are the classical shell strain measures, our approach provides us with two new strain measures which define the extension into the generalised shell theory and are responsible for the extra effects such as scale effects we are anticipating. Note also, when building the expression for the internal energy or the internal virtual work, the generalised basis cancels out upon multiplication with their duals from the stress tensor. However, the projection maps are still needed to calculate the metric of the generalised space. Note also that, as suggested earlier, the tensors \mathbf{H}_α are of

higher order and could be dropped as they come with the higher order term of $z\zeta^\alpha$.

4. The variational formulation and the corresponding equilibrium equations

Leaning on a classical principle of virtual work based on the classical *Cauchy-Green deformation tensor*, a generalised variational principle based on $\tilde{\mathbf{C}}$ (Eq. 34) can be similarly defined. With the specification of $\{\mathcal{M} \times \mathcal{L}\} \times S$, the domain of interest is not yet fully defined. What is still missing is the definition of the boundaries. Strictly speaking we have to consider a whole set of boundaries and sub-boundaries such as $(\{\partial\mathcal{M} \times \mathcal{L}\} \times S)$, $(\{\mathcal{M} \times \partial\mathcal{L}\} \times S)$, $(\{\mathcal{M} \times \mathcal{L}\} \times \partial S)$, $(\{\partial\mathcal{M} \times \partial\mathcal{L}\} \times S)$, $(\{\partial\mathcal{M} \times \mathcal{L}\} \times \partial S)$ and $(\{\partial\mathcal{M} \times \partial\mathcal{L}\} \times \partial S)$. However, for the sake of brevity and with an eye on capturing only the dominant effects, we restrict ourselves in what follows to the first type of boundaries which is $(\{\partial\mathcal{M} \times \mathcal{L}\} \times S)$.

First, we define the kinetic energy of the generalised shell space as

$$\mathcal{K} = \int_{\mathcal{M}} \int_{\mathcal{L}} \int_S \frac{1}{2} \rho_0 \dot{\tilde{\mathbf{x}}} \cdot \dot{\tilde{\mathbf{x}}} d\Sigma dL dA, \quad (35)$$

with ρ_0 denoting the density in $\{\mathcal{M} \times \mathcal{L}\} \times S$. The area element dA and the line element dL refer to the conventional shell space, i.e. its mid-surface \mathcal{M} and its thickness \mathcal{L} , respectively, while $d\Sigma$ refers to the volume, surface or length element in domain S .

Eq. (26) is now inserted in (35) and the resulting expression is explicitly integrated over the domains \mathcal{L} and S . Here again we want to restrict ourselves to the major and dominant contributions, which leaves us with the following expression

$$\begin{aligned} \mathcal{K} = & \frac{1}{2} \int_{\mathcal{M}} \left[\rho_0 h \Sigma \dot{\tilde{\mathbf{x}}} \cdot \dot{\tilde{\mathbf{x}}} + \rho_0 \frac{h^3}{12} \Sigma \dot{\tilde{\mathbf{d}}} \cdot \dot{\tilde{\mathbf{d}}} + \rho_0 h \frac{b_{(\alpha)}^3}{12} \dot{\tilde{\mathbf{a}}}_\alpha \cdot \dot{\tilde{\mathbf{a}}}_\alpha \right. \\ & \left. + \rho_0 \frac{h^3}{12} \frac{b_{(\alpha)}^3}{12} \dot{\tilde{\mathbf{b}}}_\alpha \cdot \dot{\tilde{\mathbf{b}}}_\alpha \right] dA. \end{aligned} \quad (36)$$

Here, h is the shell thickness and Σ defines the length, surface, or volume of the micro space S depending on its dimension and $b_{(\alpha)}$ is the length in the α -direction, where the bracket indicates that α is fixed and not to be treated as a free index. Obviously Σ is the product of all the $b_{(\alpha)}$ s. Note that the last two terms in the expression is the generalised contribution in the kinetic energy. They have been retained not because of their significance or magnitude but rather to give the degrees of freedom \mathbf{a}_α and \mathbf{b}_α corresponding kinetic terms. This is done for completion on the one hand, but also, on the other hand, because being very relevant in explicit type integration schemes. Indeed, in implicit type integration schemes the terms could be neglected. The only degree of freedom without a corresponding kinetic term retained in the expression is λ . This has three reasons. First, the inertia term is of the order of $O(h^5)$ which is very small. Second, the term comes in coupled form with quadratic \mathbf{d} and so again is negligible. Third, the nature of λ is different than the nature of the other degrees of freedom. The strain measures do not depend on derivatives of λ . Hence, the corresponding Euler-Lagrange equation will be an algebraic one, which suggests that λ could be eliminated. Indeed, within, say, a finite element scheme, λ could be eliminated at an element level.

The external potential in the Lagrangian form is expressed by

$$\Psi_{\text{ext}} = - \int_{\mathcal{M}} \int_{\mathcal{L}} \int_S \tilde{\mathbf{p}} \cdot \tilde{\mathbf{x}} d\Sigma dL dA - \int_{\partial\mathcal{M}_N} \int_{\mathcal{L}} \int_S \tilde{\mathbf{p}}_s \cdot \tilde{\mathbf{x}} d\Sigma dL dS, \quad (37)$$

where the generalised external body forces $\tilde{\mathbf{p}}$ and $\tilde{\mathbf{p}}_s$ act in $\{\mathcal{M} \times \mathcal{L}\} \times \mathcal{S}$ and on $\{\partial\mathcal{M}_N \times \mathcal{L}\} \times \mathcal{S}$, respectively. dS denotes a line element of the curve defining the boundary of the mid-surface $\partial\mathcal{M}$. For simplicity we have assumed the forces to be of conservative nature. Also, dS is the line element at boundary of \mathcal{M} .

Upon inserting Eq. (26), integrating over the domains \mathcal{L} and \mathcal{S} and disregarding higher order terms, one ends up with the following expression

$$\Psi_{ext} = - \int_{\mathcal{M}} (\mathbf{p} \cdot \mathbf{x} + \mathbf{l} \cdot \mathbf{d} + \mathbf{q}^\alpha \cdot \mathbf{a}_\alpha + \mathbf{r}^\alpha \cdot \mathbf{b}_\alpha) dA - \int_{\partial\mathcal{M}_N} (\mathbf{t} \cdot \mathbf{x} + \mathbf{l}_s \cdot \mathbf{d} + \mathbf{q}_s^\alpha \cdot \mathbf{a}_\alpha + \mathbf{r}_s^\alpha \cdot \mathbf{b}_\alpha) dS, \quad (38)$$

with

$$\mathbf{p} = \int_{\mathcal{L}} \int_{\mathcal{S}} \tilde{\mathbf{p}} d\Sigma dL, \quad (39)$$

$$\mathbf{l} = \int_{\mathcal{L}} \int_{\mathcal{S}} z \tilde{\mathbf{p}} d\Sigma dL, \quad (40)$$

$$\mathbf{q}^\alpha = \int_{\mathcal{L}} \int_{\mathcal{S}} \zeta^\alpha \tilde{\mathbf{p}} d\Sigma dL, \quad (41)$$

$$\mathbf{r}^\alpha = \int_{\mathcal{L}} \int_{\mathcal{S}} \zeta^\alpha z \tilde{\mathbf{p}} d\Sigma dL, \quad (42)$$

$$\mathbf{t} = \int_{\mathcal{L}} \int_{\mathcal{S}} \tilde{\mathbf{p}}_s d\Sigma dL, \quad (43)$$

$$\mathbf{l}_s = \int_{\mathcal{L}} \int_{\mathcal{S}} z \tilde{\mathbf{p}}_s d\Sigma dL, \quad (44)$$

$$\mathbf{q}_s^\alpha = \int_{\mathcal{L}} \int_{\mathcal{S}} \zeta^\alpha \tilde{\mathbf{p}}_s d\Sigma dL, \quad (45)$$

$$\mathbf{r}_s^\alpha = \int_{\mathcal{L}} \int_{\mathcal{S}} \zeta^\alpha z \tilde{\mathbf{p}}_s d\Sigma dL. \quad (46)$$

Further, we assume that the body under consideration is hyper-elastic and possesses an elastic potential Ψ_{int} represented by the stored strain energy per unit un-deformed volume $\psi(\tilde{\mathbf{C}})$. The internal potential of the stored strain energy with respect to $\tilde{\mathbf{C}}$ is then

$$\Psi_{int} = \int_{\mathcal{M}} \int_{\mathcal{L}} \int_{\mathcal{S}} \psi(\tilde{\mathbf{C}}) d\Sigma dL dA. \quad (47)$$

Now, all ingredients are defined to formulate a Lagrangian as

$$\mathcal{L} = \mathcal{K} - (\Psi_{int} + \Psi_{ext}) \quad (48)$$

such that Hamilton's principle

$$\delta \int_{t_0}^{t_1} \mathcal{L} dt = 0 \quad (49)$$

holds. Here t is the time parameter and t_0 and t_1 are the time interval boundaries.

With (36), (47) and (38), the Lagrangian reads

$$\begin{aligned} \mathcal{L} = & \frac{1}{2} \int_{\mathcal{M}} \left[\rho_0 h \Sigma \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} + \rho_0 \frac{h^3}{12} \Sigma \dot{\mathbf{d}} \cdot \dot{\mathbf{d}} + \rho_0 h \frac{b_{(\alpha)}^3}{12} \dot{\mathbf{a}}_\alpha \cdot \dot{\mathbf{a}}_\alpha + \rho_0 \frac{h^3}{12} \frac{b_{(\alpha)}^3}{12} \dot{\mathbf{b}}_\alpha \cdot \dot{\mathbf{b}}_\alpha \right] dA \\ & - \int_{\mathcal{M}} \int_{\mathcal{L}} \int_{\mathcal{S}} \psi(\tilde{\mathbf{C}}) d\Sigma dL dA + \int_{\mathcal{M}} (\mathbf{p} \cdot \mathbf{x} + \mathbf{l} \cdot \mathbf{d} + \mathbf{q}^\alpha \cdot \mathbf{a}_\alpha + \mathbf{r}^\alpha \cdot \mathbf{b}_\alpha) dA \\ & + \int_{\partial\mathcal{M}_N} (\mathbf{t} \cdot \mathbf{x} + \mathbf{l}_s \cdot \mathbf{d} + \mathbf{q}_s^\alpha \cdot \mathbf{a}_\alpha + \mathbf{r}_s^\alpha \cdot \mathbf{b}_\alpha) dS. \end{aligned} \quad (50)$$

Hamilton's principle, together with Gauss theorem and standard arguments regarding the vanishing of variations at the boundaries finally lead to the statement

$$\begin{aligned} & \int_{\mathcal{M}} \left[\rho_0 h \Sigma \ddot{\mathbf{x}} \cdot \delta \mathbf{x} + \rho_0 \frac{h^3}{12} \Sigma \ddot{\mathbf{d}} \cdot \delta \mathbf{d} + \rho_0 h \frac{b_{(\alpha)}^3}{12} \ddot{\mathbf{a}}_\alpha \cdot \delta \mathbf{a}_\alpha + \rho_0 \frac{h^3}{12} \frac{b_{(\alpha)}^3}{12} \ddot{\mathbf{b}}_\alpha \cdot \delta \mathbf{b}_\alpha \right] dA \\ & + \int_{\mathcal{M}} \int_{\mathcal{L}} \int_{\mathcal{S}} \frac{\partial \psi(\tilde{\mathbf{C}})}{\partial \tilde{\mathbf{C}}} : \delta \tilde{\mathbf{C}} d\Sigma dL dA - \int_{\mathcal{M}} (\mathbf{p} \cdot \delta \mathbf{x} + \mathbf{l} \cdot \delta \mathbf{d} + \mathbf{q}^\alpha \cdot \delta \mathbf{a}_\alpha + \mathbf{r}^\alpha \cdot \delta \mathbf{b}_\alpha) dA \\ & - \int_{\partial\mathcal{M}_N} (\mathbf{t} \cdot \delta \mathbf{x} + \mathbf{l}_s \cdot \delta \mathbf{d} + \mathbf{q}_s^\alpha \cdot \delta \mathbf{a}_\alpha + \mathbf{r}_s^\alpha \cdot \delta \mathbf{b}_\alpha) dS = 0. \end{aligned} \quad (51)$$

Inserting (34), together with (33), into the last equation leads to

$$\begin{aligned} & \int_{\mathcal{M}} \left[\rho_0 h \Sigma \ddot{\mathbf{x}} \cdot \delta \mathbf{x} + \rho_0 \frac{h^3}{12} \Sigma \ddot{\mathbf{d}} \cdot \delta \mathbf{d} + \rho_0 h \frac{b_{(\alpha)}^3}{12} \ddot{\mathbf{a}}_\alpha \cdot \delta \mathbf{a}_\alpha + \rho_0 \frac{h^3}{12} \frac{b_{(\alpha)}^3}{12} \ddot{\mathbf{b}}_\alpha \cdot \delta \mathbf{b}_\alpha \right] dA \\ & + \int_{\mathcal{M}} \mathbf{S} : \frac{1}{2} \delta \mathbf{C}_0 dA + \int_{\mathcal{M}} \mathbf{M} : \frac{1}{2} \delta \mathbf{K} dA + \int_{\mathcal{M}} \mathbf{Z}^\alpha : \frac{1}{2} \delta \mathbf{D}_\alpha dA + \int_{\mathcal{M}} \mathbf{Y}^\alpha : \frac{1}{2} \delta \mathbf{H}_\alpha dA \\ & - \int_{\mathcal{M}} (\mathbf{p} \cdot \delta \mathbf{x} + \mathbf{l} \cdot \delta \mathbf{d} + \mathbf{q}^\alpha \cdot \delta \mathbf{a}_\alpha + \mathbf{r}^\alpha \cdot \delta \mathbf{b}_\alpha) dA \\ & - \int_{\partial\mathcal{M}_N} (\mathbf{t} \cdot \delta \mathbf{x} + \mathbf{l}_s \cdot \delta \mathbf{d} + \mathbf{q}_s^\alpha \cdot \delta \mathbf{a}_\alpha + \mathbf{r}_s^\alpha \cdot \delta \mathbf{b}_\alpha) dS = 0. \end{aligned} \quad (52)$$

Here, \mathbf{S} , \mathbf{M} , \mathbf{Z}^α and \mathbf{Y}^α are resultant forces and moments which are defined as follows:

$$\mathbf{S} = \int_{\mathcal{L}} \int_{\mathcal{S}} 2(\pi_0^{M*})^{-T} \frac{\partial \psi(\tilde{\mathbf{C}})}{\partial \tilde{\mathbf{C}}} (\pi_0^{M*})^{-1} d\Sigma dL, \quad (53)$$

$$\mathbf{M} = \int_{\mathcal{L}} \int_{\mathcal{S}} 2z(\pi_0^{M*})^{-T} \frac{\partial \psi(\tilde{\mathbf{C}})}{\partial \tilde{\mathbf{C}}} (\pi_0^{M*})^{-1} d\Sigma dL, \quad (54)$$

$$\mathbf{Z}^\alpha = \int_{\mathcal{L}} \int_{\mathcal{S}} 2\zeta^\alpha (\pi_0^{M*})^{-T} \frac{\partial \psi(\tilde{\mathbf{C}})}{\partial \tilde{\mathbf{C}}} (\pi_0^{M*})^{-1} d\Sigma dL, \quad (55)$$

$$\mathbf{Y}^\alpha = \int_{\mathcal{L}} \int_{\mathcal{S}} 2z\zeta^\alpha (\pi_0^{M*})^{-T} \frac{\partial \psi(\tilde{\mathbf{C}})}{\partial \tilde{\mathbf{C}}} (\pi_0^{M*})^{-1} d\Sigma dL. \quad (56)$$

By definition these stress resultants are symmetric. In the simplest cases of a linear constitutive law the above integrals can be evaluated explicitly. In general, however, the integration is to be carried out numerically. Eq. (52) defines a variational statement which can serve as the basis for a numerical, finite element, meshfree-based or otherwise solution procedure. Note that the functional as such does not restrict the formulation to purely elastic behaviour. It is valid for any material behaviour. The definitions in Eq. (53)–(56) are the ones based on a hyper-elastic material behaviour. With modified definitions, depending on the material behaviour at hand, the functional can be applied to any type of material response.

The variational statement can serve also as a basis to derive the generalised equilibrium equations, which we want to do next. It is helpful to introduce the stress resultants in component form. In doing so we recall that the indices i, j, \dots take the values 1 and 2. For simplicity, the components in the direction z will be assigned the value 3. Accordingly, the following decompositions are in order

$$\mathbf{S} = S^{ij}(\mathbf{G}_i \otimes \mathbf{G}_j) + S^{i3}(\mathbf{G}^i \otimes \mathbf{N}) + S^{3i}(\mathbf{N} \otimes \mathbf{G}^i) + S^{33}(\mathbf{N} \otimes \mathbf{N}), \quad (57)$$

$$\mathbf{M} = M^{ij}(\mathbf{G}_i \otimes \mathbf{G}_j) + M^{i3}(\mathbf{G}^i \otimes \mathbf{N}) + M^{3i}(\mathbf{N} \otimes \mathbf{G}^i) + M^{33}(\mathbf{N} \otimes \mathbf{N}), \quad (58)$$

$$\mathbf{Z}^\alpha = Z^{\alpha ij}(\mathbf{G}_i \otimes \mathbf{G}_j) + Z^{\alpha i3}(\mathbf{G}^i \otimes \mathbf{N}) + Z^{\alpha 3i}(\mathbf{N} \otimes \mathbf{G}^i) + Z^{\alpha 33}(\mathbf{N} \otimes \mathbf{N}), \quad (59)$$

$$\mathbf{Y}^\alpha = Y^{\alpha ij}(\mathbf{G}_i \otimes \mathbf{G}_j) + Y^{\alpha i3}(\mathbf{G}^i \otimes \mathbf{N}) + Y^{\alpha 3i}(\mathbf{N} \otimes \mathbf{G}^i) + Y^{\alpha 33}(\mathbf{N} \otimes \mathbf{N}). \quad (60)$$

With the above decompositions and the definitions of all strain measures as given in (29)–(32) at hand, the functional of Eq. (52) takes the form

$$\begin{aligned}
& \int_{\mathcal{M}} \left[\rho_0 h \Sigma \ddot{\mathbf{x}} \cdot \delta \mathbf{x} + \rho_0 \frac{h^3}{12} \Sigma \ddot{\mathbf{d}} \cdot \delta \mathbf{d} + \rho_0 h \frac{b_{(x)}^3}{12} \ddot{\mathbf{a}}_x \cdot \delta \mathbf{a}_x + \rho_0 \frac{h^3}{12} \frac{b_{(x)}^3}{12} \ddot{\mathbf{b}}_x \cdot \delta \mathbf{b}_x \right] dA \\
& + \int_{\mathcal{M}} \left[\left(S^{ij} \mathbf{x}_j + S^{i3} \mathbf{d} + M^{ij} \mathbf{d}_j + 2M^{i3} \lambda \mathbf{d} + Z^{zij} \mathbf{a}_{xj} + Z^{zi3} \mathbf{b}_x + Y^{ij} \mathbf{b}_{xj} \right) \cdot \delta \mathbf{x}_i \right. \\
& + \left(S^{i3} \mathbf{x}_i + S^{33} \mathbf{d} + M^{i3} (\mathbf{d}_i + 2\lambda \mathbf{x}_i) + 4M^{33} \lambda \mathbf{d} + Z^{zi3} \mathbf{a}_{xi} + Z^{z33} \mathbf{b}_x + Y^{zi3} \right. \\
& \times (2\lambda \mathbf{a}_{xi} + \mathbf{b}_{xi}) + Y^{z33} 2\lambda \mathbf{b}_x \cdot \delta \mathbf{d} + \left(M^{ij} \mathbf{x}_j + M^{i3} \mathbf{d} + Y^{zij} \mathbf{a}_{xj} + Y^{zi3} \mathbf{b}_x \right) \cdot \delta \mathbf{d}_i \\
& + \left(2M^{i3} \mathbf{x}_i \cdot \mathbf{d} + 2M^{33} \mathbf{d} \cdot \mathbf{d} + Y^{zi3} 2\mathbf{a}_{xi} \cdot \mathbf{d} + Y^{z33} 2\mathbf{d} \cdot \mathbf{b}_x \right) \delta \lambda \\
& + \left(Z^{zij} \mathbf{x}_j + Z^{zi3} \mathbf{d} + Y^{zij} \mathbf{d}_j + 2Y^{zi3} \lambda \mathbf{d} \right) \cdot \delta \mathbf{a}_{xi} \\
& + \left(Z^{zi3} \mathbf{x}_i + Z^{z33} \mathbf{d} + Y^{zi3} \mathbf{d}_i + 2Y^{z33} \lambda \mathbf{d} \right) \cdot \delta \mathbf{b}_x \\
& \left. + \left(Y^{zij} \mathbf{x}_j + Y^{zi3} \mathbf{d} \right) \cdot \delta \mathbf{b}_{xi} \right] dA \\
& - \int_{\mathcal{M}} (\mathbf{p} \cdot \delta \mathbf{x} + \mathbf{l} \cdot \delta \mathbf{d} + \mathbf{q}^\alpha \cdot \delta \mathbf{a}_\alpha + \mathbf{r}^\alpha \cdot \delta \mathbf{b}_\alpha) dA \\
& - \int_{\partial \mathcal{M}_N} (\mathbf{t} \cdot \delta \mathbf{x} + \mathbf{l}_s \cdot \delta \mathbf{d} + \mathbf{q}_s^\alpha \cdot \delta \mathbf{a}_\alpha + \mathbf{r}_s^\alpha \cdot \delta \mathbf{b}_\alpha) dS = 0. \quad (61)
\end{aligned}$$

Now Gauss theorem, together with standard arguments of variational calculus, provide us with the Euler–Lagrange equations of the above functional which read:

$$\rho_0 h \Sigma \ddot{\mathbf{x}} = \frac{1}{\sqrt{G}} \left[\sqrt{G} \left(S^{ij} \mathbf{x}_j + S^{i3} \mathbf{d} + M^{ij} \mathbf{d}_j + 2M^{i3} \lambda \mathbf{d} + Z^{zij} \mathbf{a}_{xj} + Z^{zi3} \mathbf{b}_x + Y^{ij} \mathbf{b}_{xj} \right) \right]_i + \mathbf{p}, \quad (62)$$

$$\rho_0 \frac{h^3}{12} \Sigma \ddot{\mathbf{d}} = - \left[S^{i3} \mathbf{x}_i + S^{33} \mathbf{d} + M^{i3} (\mathbf{d}_i + 2\lambda \mathbf{x}_i) + 4M^{33} \lambda \mathbf{d} + Z^{zi3} \mathbf{a}_{xi} + Z^{z33} \mathbf{b}_x + Y^{zi3} (2\lambda \mathbf{a}_{xi} + \mathbf{b}_{xi}) + Y^{z33} 2\lambda \mathbf{b}_x \right] + \frac{1}{\sqrt{G}} \left[\sqrt{G} \left(M^{ij} \mathbf{x}_j + M^{i3} \mathbf{d} + Y^{zij} \mathbf{a}_{xj} + Y^{zi3} \mathbf{b}_x \right) \right]_i + \mathbf{l}, \quad (63)$$

$$2M^{i3} \mathbf{x}_i \cdot \mathbf{d} + 2M^{33} \mathbf{d} \cdot \mathbf{d} + Y^{zi3} 2\mathbf{a}_{xi} \cdot \mathbf{d} + Y^{z33} 2\mathbf{d} \cdot \mathbf{b}_x = 0, \quad (64)$$

$$\rho_0 h \frac{b_{(x)}^3}{12} \ddot{\mathbf{a}}_x = \frac{1}{\sqrt{G}} \left[\sqrt{G} \left(Z^{zij} \mathbf{x}_j + Z^{zi3} \mathbf{d} + Y^{zij} \mathbf{d}_j + 2Y^{zi3} \lambda \mathbf{d} \right) \right]_i + \mathbf{q}^\alpha \quad (65)$$

$$\rho_0 \frac{h^3}{12} \frac{b_{(x)}^3}{12} \ddot{\mathbf{b}}_x = - \left(Z^{zi3} \mathbf{x}_i + Z^{z33} \mathbf{d} + Y^{zi3} \mathbf{d}_i + 2Y^{z33} \lambda \mathbf{d} \right) + \frac{1}{\sqrt{G}} \left[\sqrt{G} \left(Y^{zij} \mathbf{x}_j + Y^{zi3} \mathbf{d} \right) \right]_i + \mathbf{r}^\alpha. \quad (66)$$

These are five equilibrium equations for the generalised shell. The first equation is the standard linear momentum equation extended by various terms which relate to the new generalised stress resultants. The second is the angular momentum equation, extended too by these terms. The third equation is a higher order equilibrium equation which relates to the degree of freedom λ . It describes a higher order equilibrium in the z direction and is modified by some generalised terms which would be absent in a classical version of the theory. The last two equations are purely generalised ones and would be completely absent in a classical version of the shell theory. Note also that the term $1/\sqrt{G} [\sqrt{G}(\cdot)]_i$ is nothing but the divergence operator applied to the bracketed expression.

We recall also that the integration over the micro-continuum \mathcal{S} in Eqs. (53)–(56) provides the micro-structure characterising internal length scale parameters and, so, scale effects are automatically accounted for. Specifically, the coordinates of the micro-space ζ^α are defined over the intervals $[-\frac{b_x}{2}, \frac{b_x}{2}]$, where b_x are the internal length scale parameters associated with the different dimensions of \mathcal{S} .

The above field equations are complemented with the corresponding Dirichlet boundary conditions

$$\mathbf{x} = \mathbf{x}_u, \quad \mathbf{d} = \mathbf{d}_u, \quad \mathbf{a}_\alpha = \mathbf{a}_{\alpha|u}, \quad \mathbf{b}_\alpha = \mathbf{b}_{\alpha|u} \quad \text{on } \partial \mathcal{M}_D, \quad (67)$$

with $\partial \mathcal{M}_D = \partial \mathcal{M} \setminus \partial \mathcal{M}_N$. Unless there is a physical indication as to the possible values of $\mathbf{a}_{\alpha|u}$ and $\mathbf{b}_{\alpha|u}$, homogenous boundary conditions for these quantities will be assumed.

The Neumann boundary conditions on $\partial \mathcal{M}_N$, which are the outcome of the evaluation of Hamilton's principle, read:

$$\left[\sqrt{G} \left(S^{ij} \mathbf{x}_j + S^{i3} \mathbf{d} + M^{ij} \mathbf{d}_j + 2M^{i3} \lambda \mathbf{d} + Z^{zij} \mathbf{a}_{xj} + Z^{zi3} \mathbf{b}_x + Y^{ij} \mathbf{b}_{xj} \right) \right] v_i = \mathbf{t} \quad (68)$$

$$\left[\sqrt{G} \left(M^{ij} \mathbf{x}_j + M^{i3} \mathbf{d} + Y^{zij} \mathbf{a}_{xj} + Y^{zi3} \mathbf{b}_x \right) \right] v_i = \mathbf{l}_s \quad (69)$$

$$\left[\sqrt{G} \left(Z^{zij} \mathbf{x}_j + Z^{zi3} \mathbf{d} + Y^{zij} \mathbf{d}_j + 2Y^{zi3} \lambda \mathbf{d} \right) \right] v_i = \mathbf{q}_s^\alpha \quad (70)$$

$$\left[\sqrt{G} \left(Y^{zij} \mathbf{x}_j + Y^{zi3} \mathbf{d} \right) \right] v_i = \mathbf{r}_s^\alpha \quad (71)$$

where v_i are the components of the normal at the boundary $\mathbf{v} = v_i \mathbf{G}^i$.

Remark. It should be noted that the final definition of the volume elements through the metric \sqrt{G} in normalised by the volume (or surface or length) of the micro continuum, such that the integration process provides us with the correct values of volumes or surfaces etc. Alternatively such a normalisation process can be achieved by including it in the definition of the stress resultants (53)–(56) and that of the resultant forces. The definitions then are given as average values over the micro volumes (surfaces or lengths). Another equivalent way is to define from the outset the internal potential (Eq. (47)) normalised (divided) by the micro volume (surface or length).

5. A higher gradient shell theory

In the preceding sections a complete shell theory has been presented with altogether 7 classical degrees of freedom and a further family of vectors \mathbf{a}_α and \mathbf{b}_α , which define the generalised degrees of freedom the number of which depends on the selected dimension of the micro space. In what follows we would like to reduce the number of these extra degrees of freedom by presenting a shell theory which preserves most of the features of the theory presented so far without increasing the number of degrees of freedom. This comes at the price of increasing the order of derivatives involved such that the shell theory becomes a higher gradient theory. The starting point is Eq. (26). With the choice of

$$\left[\mathbf{a}_\alpha(\vartheta^k, t) + z \mathbf{b}_\alpha(\vartheta^k, t) \right] = \frac{\partial}{\partial \vartheta^\alpha} \left[\mathbf{x}(\vartheta^k, t) + z \mathbf{d}(\vartheta^k, t) \right], \quad (72)$$

we can eliminate the extra degrees of freedom. However, the choice restricts the dimension of the extra micro space to two or less since the dimension of the base continuum (the shell surface) is itself two. This restriction may be considered as sufficient in most practical cases. The above choice results in

$$\mathbf{a}_\alpha(\vartheta^k, t) = \frac{\partial}{\partial \vartheta^\alpha} \mathbf{x}(\vartheta^k, t), \quad (73)$$

$$\mathbf{b}_\alpha(\vartheta^k, t) = \frac{\partial}{\partial \vartheta^\alpha} \mathbf{d}(\vartheta^k, t). \quad (74)$$

With the above choices the deformation gradient takes the form

$$\tilde{\mathbf{F}} = (\mathbf{x}_i + (Z + Z^2 \lambda) \mathbf{d}_i + Z^2 \lambda_i \mathbf{d} + \zeta^\alpha \mathbf{x}_{,\alpha i} + Z \zeta^\alpha \mathbf{d}_{,\alpha i}) \otimes \tilde{\mathbf{G}}^i + [(1 + 2Z\lambda) \mathbf{d} + \zeta^\alpha \mathbf{d}_{,\alpha}] \otimes \tilde{\mathbf{N}} + (\mathbf{x}_{,\alpha} + Z \mathbf{d}_{,\alpha}) \otimes \tilde{\mathbf{I}}^\alpha. \quad (75)$$

With this expression at hand the strain measures of the shell theory can be derived. Indeed similar to the expressions given in Eqs. (29)–(32), the modified strain measures read:

$$\mathbf{C}_0 = \mathbf{x}_i \cdot \mathbf{x}_j (\mathbf{G}^i \otimes \mathbf{G}^j) + \mathbf{x}_i \cdot \mathbf{d} (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) + \mathbf{d} \cdot \mathbf{d} (\mathbf{N} \otimes \mathbf{N}), \quad (76)$$

$$\mathbf{K} = (\mathbf{x}_i \cdot \mathbf{d}_j + \mathbf{d}_i \cdot \mathbf{x}_j) (\mathbf{G}^i \otimes \mathbf{G}^j) + (\mathbf{d}_i \cdot \mathbf{d} + 2\lambda \mathbf{x}_i \cdot \mathbf{d}) (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) + 4\lambda \mathbf{d} \cdot \mathbf{d} (\mathbf{N} \otimes \mathbf{N}), \quad (77)$$

$$\mathbf{D}_\alpha = (\mathbf{x}_i \cdot \mathbf{x}_{,\alpha j} + \mathbf{x}_{,\alpha i} \cdot \mathbf{x}_j) (\mathbf{G}^i \otimes \mathbf{G}^j) + (\mathbf{x}_{,\alpha i} \cdot \mathbf{d} + \mathbf{x}_{,\alpha i} \cdot \mathbf{d}) (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) + 2\mathbf{d} \cdot \mathbf{d}_{,\alpha} (\mathbf{N} \otimes \mathbf{N}), \quad (78)$$

$$\mathbf{H}_\alpha = (\mathbf{x}_i \cdot \mathbf{d}_{,\alpha j} + \mathbf{x}_{,\alpha j} \cdot \mathbf{d}_i + \mathbf{x}_{,\alpha i} \cdot \mathbf{d}_j + \mathbf{x}_{,\alpha j} \cdot \mathbf{d}_i) (\mathbf{G}^i \otimes \mathbf{G}^j) + (2\lambda \mathbf{x}_{,\alpha i} \cdot \mathbf{d} + \mathbf{d} \cdot \mathbf{d}_{,\alpha i} + \mathbf{d}_i \cdot \mathbf{d}_{,\alpha}) (\mathbf{G}^i \otimes \mathbf{N} + \mathbf{N} \otimes \mathbf{G}^i) + 4\lambda \mathbf{d} \cdot \mathbf{d}_{,\alpha} (\mathbf{N} \otimes \mathbf{N}). \quad (79)$$

The external potential becomes:

$$\Psi_{ext} = - \int_{\mathcal{M}} (\mathbf{p} \cdot \mathbf{x} + \mathbf{l} \cdot \mathbf{d} + \mathbf{q}^\alpha \cdot \mathbf{x}_{,\alpha} + \mathbf{r}^\alpha \cdot \mathbf{d}_{,\alpha}) dA - \int_{\partial \mathcal{M}_N} (\mathbf{t} \cdot \mathbf{x} + \mathbf{l}_s \cdot \mathbf{d} + \mathbf{q}_s^\alpha \cdot \mathbf{x}_{,\alpha} + \mathbf{r}_s^\alpha \cdot \mathbf{d}_{,\alpha}) dS \quad (80)$$

and the kinetic energy takes now the more complex form

$$\mathcal{K} = \frac{1}{2} \int_{\mathcal{M}} \left[\rho_0 h \Sigma \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} + \rho_0 \frac{h^3}{12} \Sigma \dot{\mathbf{d}} \cdot \dot{\mathbf{d}} + \rho_0 h \frac{b^{(3)}}{12} \dot{\mathbf{x}}_{,\alpha} \cdot \dot{\mathbf{x}}_{,\alpha} + \rho_0 \frac{h^3}{12} \frac{b^{(3)}}{12} \dot{\mathbf{d}}_{,\alpha} \cdot \dot{\mathbf{d}}_{,\alpha} \right] dA. \quad (81)$$

However, since the first two terms in the above expression already provide a kinetic contribution related to the degrees of freedom and with the fact that the last two terms are small in magnitude, hitherto these last two terms will be neglected.

The definition of the stress resultants remains unchanged and so the evaluation of Hamilton's principle now results in the following expression, which is the counter part to the functional in Eq. (61),

$$\begin{aligned} & \int_{\mathcal{M}} \left[\rho_0 h \Sigma \ddot{\mathbf{x}} \cdot \delta \mathbf{x} + \rho_0 \frac{h^3}{12} \Sigma \ddot{\mathbf{d}} \cdot \delta \mathbf{d} \right] dA \\ & + \int_{\mathcal{M}} \left[\left(S^{ij} \mathbf{x}_j + S^{i3} \mathbf{d} + M^{ij} \mathbf{d}_j + 2M^{i3} \lambda \mathbf{d} + Z^{\alpha ij} \mathbf{x}_{,\alpha j} + Z^{\alpha i3} \mathbf{d}_{,\alpha} + Y^{ij} \mathbf{d}_{,\alpha j} \right) \cdot \delta \mathbf{x}_i + \left(S^{i3} \mathbf{x}_i + S^{33} \mathbf{d} + M^{i3} (\mathbf{d}_i + 2\lambda \mathbf{x}_i) + 4M^{33} \lambda \mathbf{d} + Z^{\alpha i3} \mathbf{x}_{,\alpha i} + Z^{\alpha 33} \mathbf{d}_{,\alpha} + Y^{\alpha i3} (2\lambda \mathbf{x}_{,\alpha i} + \mathbf{d}_{,\alpha i}) + Y^{\alpha 33} 2\lambda \mathbf{d}_{,\alpha} \right) \cdot \delta \mathbf{d}_i \right. \\ & + \left(M^{ij} \mathbf{x}_j + M^{i3} \mathbf{d} + Y^{\alpha ij} \mathbf{x}_{,\alpha j} + Y^{\alpha i3} \mathbf{d}_{,\alpha} \right) \cdot \delta \mathbf{d}_i \\ & + \left(2M^{i3} \mathbf{x}_i \cdot \mathbf{d} + 2M^{33} \mathbf{d} \cdot \mathbf{d} + Y^{\alpha i3} 2\mathbf{x}_{,\alpha i} \cdot \mathbf{d} + Y^{\alpha 33} 2\mathbf{d} \cdot \mathbf{d}_{,\alpha} \right) \delta \lambda \\ & + \left(Z^{\alpha ij} \mathbf{x}_j + Z^{\alpha i3} \mathbf{d} + Y^{\alpha ij} \mathbf{d}_j + 2Y^{\alpha i3} \lambda \mathbf{d} \right) \cdot \delta \mathbf{x}_{,\alpha i} \\ & + \left(Z^{\alpha i3} \mathbf{x}_i + Z^{\alpha 33} \mathbf{d} + Y^{\alpha i3} \mathbf{d}_i + 2Y^{\alpha 33} \lambda \mathbf{d} \right) \cdot \delta \mathbf{d}_{,\alpha} \\ & + \left(Y^{\alpha ij} \mathbf{x}_j + Y^{\alpha i3} \mathbf{d} \right) \cdot \delta \mathbf{d}_{,\alpha i} \Big] dA \\ & - \int_{\mathcal{M}} (\mathbf{p} \cdot \delta \mathbf{x} + \mathbf{l} \cdot \delta \mathbf{d} + \mathbf{q}^\alpha \cdot \delta \mathbf{x}_{,\alpha} + \mathbf{r}^\alpha \cdot \delta \mathbf{d}_{,\alpha}) dA \\ & - \int_{\partial \mathcal{M}_N} (\mathbf{t} \cdot \delta \mathbf{x} + \mathbf{l}_s \cdot \delta \mathbf{d} + \mathbf{q}_s^\alpha \cdot \delta \mathbf{x}_{,\alpha} + \mathbf{r}_s^\alpha \cdot \delta \mathbf{d}_{,\alpha}) dS = 0. \end{aligned} \quad (82)$$

This functional can serve as a starting point for a numerical formulation. Indeed the numerical treatment in Section (6) is based on it. It is worthwhile, however, to write down the resulting Euler–Lagrange equations. The latter can be derived in a standard way by applying Gauss theorem twice and by making the standard arguments of calculus of variation. One achieves:

$$\begin{aligned} \rho_0 h \Sigma \ddot{\mathbf{x}} &= \frac{1}{\sqrt{G}} \left[\sqrt{G} (S^{ij} \mathbf{x}_j + S^{i3} \mathbf{d} + M^{ij} \mathbf{d}_j + 2M^{i3} \lambda \mathbf{d} + Z^{\alpha ij} \mathbf{x}_{,\alpha j} + Z^{\alpha i3} \mathbf{d}_{,\alpha} + Y^{ij} \mathbf{d}_{,\alpha j}) \right]_i \\ & - \frac{1}{\sqrt{G}} \left[\sqrt{G} (Z^{\alpha ij} \mathbf{x}_j + Z^{\alpha i3} \mathbf{d} + Y^{\alpha ij} \mathbf{d}_j + 2Y^{\alpha i3} \lambda \mathbf{d}) \right]_{,\alpha i} + \mathbf{p} + \mathbf{q}_s^\alpha, \\ \rho_0 \frac{h^3}{12} \Sigma \ddot{\mathbf{d}} &= - \left[S^{i3} \mathbf{x}_i + S^{33} \mathbf{d} + M^{i3} (\mathbf{d}_i + 2\lambda \mathbf{x}_i) + 4M^{33} \lambda \mathbf{d} + Z^{\alpha i3} \mathbf{x}_{,\alpha i} + Z^{\alpha 33} \mathbf{d}_{,\alpha} + Y^{\alpha i3} \right. \\ & \times (2\lambda \mathbf{x}_{,\alpha i} + \mathbf{d}_{,\alpha i}) + Y^{\alpha 33} 2\lambda \mathbf{d}_{,\alpha} \Big] \\ & + \frac{1}{\sqrt{G}} \left[\sqrt{G} (M^{ij} \mathbf{x}_j + M^{i3} \mathbf{d} + Y^{\alpha ij} \mathbf{x}_{,\alpha j} + Y^{\alpha i3} \mathbf{d}_{,\alpha}) \right]_i \\ & + \frac{1}{\sqrt{G}} \left[\sqrt{G} (Z^{\alpha i3} \mathbf{x}_i + Z^{\alpha 33} \mathbf{d} + Y^{\alpha i3} \mathbf{d}_i + 2Y^{\alpha 33} \lambda \mathbf{d}) \right]_{,\alpha} \\ & - \frac{1}{\sqrt{G}} \left[\sqrt{G} (Y^{\alpha ij} \mathbf{x}_j + Y^{\alpha i3} \mathbf{d}) \right]_{,\alpha i} = \mathbf{l} + \mathbf{r}_s^\alpha, \\ 2M^{i3} \mathbf{x}_i \cdot \mathbf{d} + 2M^{33} \mathbf{d} \cdot \mathbf{d} + Y^{\alpha i3} 2\mathbf{x}_{,\alpha i} \cdot \mathbf{d} + Y^{\alpha 33} 2\lambda \mathbf{d} \cdot \mathbf{d}_{,\alpha} &= 0. \end{aligned} \quad (83)$$

The above equilibrium equations are complemented with the Dirichlet boundary conditions

$$\mathbf{x} = \mathbf{x}_u \quad \text{on } \partial \mathcal{M}_D \quad \text{and} \quad \mathbf{d} = \mathbf{d}_u \quad \text{on } \partial \mathcal{M}_D, \quad (86a, b)$$

$$\frac{\partial \mathbf{x}}{\partial \theta^\alpha} v_\alpha = \mathbf{h}_u \quad \text{on } \partial \mathcal{M}_D \quad \text{and} \quad \frac{\partial \mathbf{d}}{\partial \theta^\alpha} v_\alpha = \mathbf{g}_u \quad \text{on } \partial \mathcal{M}_D, \quad (87a)$$

together with the Neumann boundary conditions on $\partial \mathcal{M}_N$:

$$\left[\sqrt{G} (S^{ij} \mathbf{x}_j + S^{i3} \mathbf{d} + M^{ij} \mathbf{d}_j + 2M^{i3} \lambda \mathbf{d} + Z^{\alpha ij} \mathbf{x}_{,\alpha j} + Z^{\alpha i3} \mathbf{d}_{,\alpha} + Y^{ij} \mathbf{d}_{,\alpha j}) \right] v_i - \left[\sqrt{G} (Z^{\alpha ij} \mathbf{x}_j + Z^{\alpha i3} \mathbf{d} + Y^{\alpha ij} \mathbf{d}_j + 2Y^{\alpha i3} \lambda \mathbf{d}) \right]_{,\alpha i} v_\alpha = \mathbf{t}, \quad (88)$$

$$\sqrt{G} (Z^{\alpha ij} \mathbf{x}_j + Z^{\alpha i3} \mathbf{d} + Y^{\alpha ij} \mathbf{d}_j + 2Y^{\alpha i3} \lambda \mathbf{d}) v_i = \mathbf{q}_s^\alpha, \quad (89)$$

$$\left[\sqrt{G} (M^{ij} \mathbf{x}_j + M^{i3} \mathbf{d} + Y^{\alpha ij} \mathbf{x}_{,\alpha j} + Y^{\alpha i3} \mathbf{d}_{,\alpha}) \right] v_i + \left[\sqrt{G} (Z^{\alpha i3} \mathbf{x}_i + Z^{\alpha 33} \mathbf{d} + Y^{\alpha i3} \mathbf{d}_i + 2Y^{\alpha 33} \lambda \mathbf{d}) \right] v_\alpha - \left[\sqrt{G} (Y^{\alpha ij} \mathbf{x}_j + Y^{\alpha i3} \mathbf{d}) \right]_{,\alpha i} v_\alpha = \mathbf{l}_s, \quad (90)$$

$$\sqrt{G} (Y^{\alpha ij} \mathbf{x}_j + Y^{\alpha i3} \mathbf{d}) v_i = \mathbf{r}_s^\alpha, \quad (91)$$

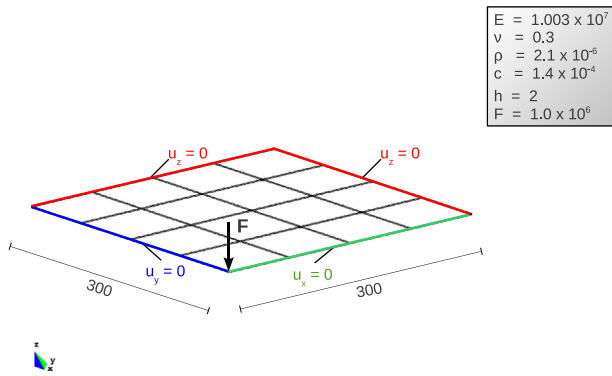


Fig. 2. problem definition of a square sheet subjected to perpendicular point force.

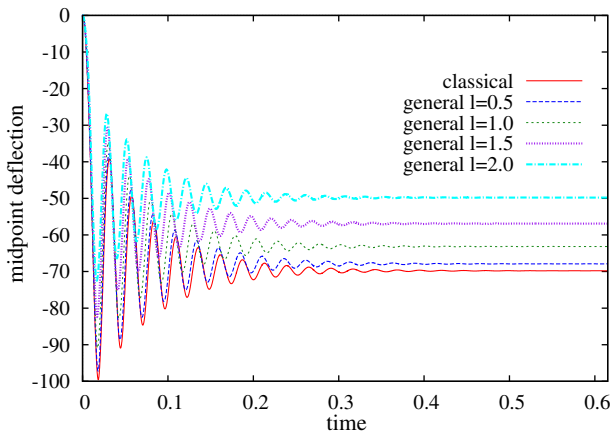


Fig. 3. midpoint deflection over time illustrating elastic size- scale effects controlled by the magnitude of the internal length scale l .

where v_i or v_α are again the components of the normal at the boundary $\mathbf{v} = v_\alpha \mathbf{G}^\alpha$. In performing the Gauss theorem we have assumed that the dimension of the micro space is the same as that of the surface, that is α takes the values 1 and 2. In case of a choice of a different dimension, the process is to be modified accordingly. However, the approach as such remains exactly the same.

Now, the above field equations have been derived via Hamilton's principle and so damping terms are not involved. However, it is straightforward to expand these equations to include velocity dependent terms of the form $ch\Sigma\dot{\mathbf{x}}$ and $c\frac{h^3}{12}\Sigma\dot{\mathbf{d}}$, with c being some damping parameter.

6. Numerical example

For illustrative purposes only we consider one numerical example with the aim to qualitatively demonstrate size-scale effects captured by the generalised shell theory. The details of the numerical approach and further numerical studies are to be found elsewhere (Sansour et al., in press). The numerical results are compared with a classical Green strain tensor-based formulation, (Skatulla et al., 2008). We make use of the classical hyperelastic Saint–Venant–Kirchhoff constitutive law which involves as material parameters the Young's modulus E and Poisson's ratio ν . For modelling purposes the strain gradient-enriched shell theory is implemented into a moving least square (MLS)-based meshfree code (Belytschko et al., 1994; Liu et al., 1995). The dynamical modelling utilizes an implicit time integration scheme based on the midpoint rule. The Dirichlet boundary condition are enforced by the modified boundary collocation method (Wagner et al., 2000). The micro-continuum S attached to each macroscopic point

$\mathbf{X} + \mathbf{Z} \in \mathcal{M} \times \mathcal{L}$ is chosen to be one-dimensional with the associated micro-vector being defined in Eqs. (73) and (74) to be parallel to the sheets normal vectors in the un-deformed configuration; in Eq. (72); the index α takes one value which is 3:

$$\mathbf{a}_3(\vartheta^k, t) = \frac{\partial}{\partial \vartheta^3} \mathbf{x}(\vartheta^k, t), \quad \mathbf{b}_3(\vartheta^k, t) = \frac{\partial}{\partial \vartheta^3} \mathbf{d}(\vartheta^k, t). \quad (92)$$

The internal length scale parameter associated with the respective micro-space dimension is l and is kept constant throughout the entire macro-space $\mathcal{M} \times \mathcal{L}$. The numerical integration over the micro-space is carried out with the help of the Gauss quadrature.

The following example, depicted in Fig. 2, is a square sheet subjected to a perpendicular point force in the center of the sheet. Exploiting its symmetry, only one quarter of the problem domain is modelled and discretised by 25 uniformly spaced particles. At its boundaries the vertical displacements are set to zero, however, in-plane displacements are possible. The loading rate is chosen as 1.0×10^5 for a given force unit per time unit.

Due to the rapid load application the sheet is excited to swing but the damping provides that the static solution $u_z = -69.79$ is obtained at time $t \approx 0.45$ as shown in Fig. 3. The red curve indicates the classical Green² strain-based solution and the curves in dark-blue, green, purple and sky-blue illustrate the dynamic deformation behaviour predicted by the generalised shell theory with increasing internal length scale parameter l .

Clearly, for larger values of the internal length l , the sheet behaves stiffer influencing the deflection amplitude as well as the swinging frequency; the amplitude is decreasing whereas the frequency is increasing. Moreover, as the static solution is approached, we find an increase in frequency over time which is more rapid for larger length scale parameters. This behaviour is consistent with the increase in stiffness of the sheet due the higher-order strain contributions which become more dominant for larger l 's.

7. Conclusion

The presented generalised shell theory constitutes the direct adaption of the fully three- dimensional strain gradient approach (Sansour et al., 2009). Albeit it bears similarities to the latter, the shell-specific kinematics leads to new generalised strain measures which, however, can be directly applied to conventional three-dimensional constitutive laws. The influence of the micro-structure, in particular its orientation, is linked to the strain gradient contributions and its associated internal length scale parameters. In this way, it naturally enters the resulting macroscopic material behaviour without additional constitutive parameters besides the geometrical specifications of the micro-continuum.

While the present paper focuses on a generalised theory, it merely alludes to potential areas of application exemplified by one numerical example. The authors do acknowledge the importance of additional experimental verification knowing that it is indeed still an ongoing area of research in the fields of mechanics and physics. In particular, the magnitude of the internal length scale parameters in the proposed model in relation to the actual characteristic lengths of the material under consideration requires attention. Moreover, in order to extend the theory's range of application, it is worthwhile to explore less trivial micro-space metrics as well as higher-order strain and stress tensors embedded in an extended space with corresponding constitutive laws specifically tailored to it. The present paper do provide the framework to do so.

² For interpretation of color in Fig. 3 the reader is referred to the web version of this article.

References

- Aifantis, E.C., 1999. Strain gradient interpretation of size effects. *Int. J. Fracture* 95, 299–314.
- Akarapu, S., Zbib, H.M., 2006. Numerical analysis of plane cracks in strain-gradient elastic materials. *Int. J. Fracture* 141, 403–430.
- Arciniega, R.A., Reddy, J.N., 2007. Tensor-based finite element formulation for geometrically nonlinear analysis of shell structures. *Comput. Methods Appl. Mech. Eng.* 196, 1048–1073.
- Areias, P.M.A., Song, J.H., Belytschko, T., 2005. A finite-strain quadrilateral shell element based on discrete kirchhoff constraints. *Int. J. Numer. Methods Eng.* 64, 1166–1206.
- Basar, Y., Ding, Y., 1990. Finite-rotation elements for the nonlinear analysis of thin shell structures. *Int. J. Solids Struct.* 26, 83–97.
- Belytschko, T., Gu, L., Lu, Y.Y., 1994. Fracture and crack growth by element-free galerkin methods. *Model. Simul. Mater. Sci. Eng.* 2, 519–534.
- Betsch, P., Gruttmann, F., Stein, E., 1996. A 4-node finite shell element for the implementation of general hyperelastic 3d-elasticity at finite strains. *Comput. Methods Appl. Mech. Eng.* 130, 57–79.
- Bischoff, M., Ramm, E., 1997. Shear deformable shell elements for large strains and rotations. *Int. J. Numer. Methods Eng.* 40, 4427–4449.
- Buechter, N., Ramm, E., Roehl, D., 1994. 3-dimensional extension of nonlinear shell formulation based on the enhanced assumed strain concept. *Int. J. Numer. Methods Eng.* 37, 2551G–2568.
- Chrosielewski, J., Makowski, J., Stumpf, H., 1992. Genuinely resultant shell finite elements accounting for geometric and material nonlinearity. *Int. J. Numer. Methods Eng.* 35, 63–94.
- Cirak, F., Ortiz, M., Schroeder, P., 2000. Subdivision surfaces: a new paradigm for thin-shell finite-element analysis. *Int. J. Numer. Methods Eng.* 47, 2039–2072.
- Cohen, H., DeSilva, K.N., 1966. Nonlinear theory of elastic directed surfaces. *J. Math. Phys.* 7, 960.
- Dillard, T., Forest, S., Ienyyb, P., 2006. Micromorphic continuum modelling of the deformation and fracture behaviour of nickel foams. *Eur. J. Mech. A/Solids* 25, 526–549.
- Dung, N.T., Wells, G.N., 2008. Geometrically nonlinear formulation for thin shells without rotation degrees of freedom. *Comput. Methods Appl. Mech. Eng.* 197, 2778–2788.
- Ericksen, J.L., Truesdell, C., 1957. Exact theory of stress and strain in rods and shells. *Arch. Ration. Mech. Anal.* 1, 295–323.
- Eringen, A.C., 1999. *Microcontinuum Field Theories I: Foundations and Solids*. Springer, New York.
- Green, A.E., Naghdi, P.M., Wainwright, W.L., 1965. A general theory of a cosserat surface. *Arch. Rat. Mech. Anal.* 20, 287–308.
- Ibrahimbegovic, A., Brank, B., Courtois, P., 1235. Stress resultant geometrically exact form of classical shell model and vector-like parametrization of constrained finite rotations. *Int. J. Numer. Methods Eng.* 52, 1235–1252.
- Klinkel, S., Gruttmann, F., Wagner, W., 2008. A mixed shell formulation accounting for thickness strains and finite strain 3d material models. *Int. J. Numer. Methods Eng.* 74, 945–970.
- Koiter, W.T., 1963. Buckling of cylindrical shells under axial compression. In: *Proceedings of the Royal Netherlands Academy of Science, Series B*, vol. 66, Amsterdam.
- Kouznetsova, V., Geers, M.G.D., Brekelmans, W.A.M., 1235. Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenization scheme. *Int. J. Numer. Methods Eng.* 54, 1235–1260.
- Kulikov, G.M., Plotnikova, S.V., 2002. Simple and effective elements based upon timoshenko-mindlin shell theory. *Comput. Methods Appl. Mech. Eng.* 191, 1173–1187.
- Kumar, R.S., McDowell, D.L., 2004. Generalized continuum modeling of 2-d periodic cellular solids. *Int. J. Solids Struct.* 41, 7399–7422.
- Larsson, R., Diebels, S., 2006. A second-order homogenization procedure for multi-scale analysis based on micropolar kinematics. *Int. J. Numer. Methods Eng.* 69, 2485–2512.
- Lazar, M., Maugin, G., Aifantis, E.C., 2006. Dislocations in second strain gradient elasticity. *Int. J. Solids Struct.* 43, 1787–1817.
- Libai, A., Simmonds, J.G., 1983. *Advances in Applied Mechanics. Nonlinear elastic shell theory*. Academic Press, New York, pp. 271–371.
- Liu, W.K., Chen, Y., 1995. Wavelet and multiple scale reproducing kernel methods. *J. Numer. Methods Fluids* 21, 901–931.
- Manzaria, M.T., Regueiro, R.A., 2005. Gradient plasticity modeling of geomaterials in a meshfree environment. Part I: Theory and variational formulation. *Mech. Res. Commun.* 32, 536–546.
- Merlini, T., Morandini, M., 2011. Computational shell mechanics by helicoidal modeling. I: Theory. *J. Mech. Mater. Struct.* 6, 659–692.
- Naghdi, P.M., 1972. *The theory of shells*. Handbuch der Physik. Springer-Verlag, Berlin, Heidelberg, New York, pp. 301–317.
- Ohashi, T., Kawamukai, M., Zbib, H.M., 1307. Multiscale modeling of size effects in fcc crystals: discrete dislocation dynamics and density based gradient crystal plasticity. *Philos. Mag.* 87, 1307–1326.
- Papargyri-Beskou, S., Beskos, D.E., 2009. Stability analysis of gradient elastic circular cylindrical thin shells. *Int. J. Eng. Sci.* 47, 1379–1385.
- Parisch, H., 1995. A continuum based shell theory for nonlinear applications. *Int. J. Numer. Methods Eng.* 38, 1855–1883.
- Pietraszkiewicz, W., 1974. Lagrangian nonlinear theory of shells. *Arch. Mech.* 26, 221–228.
- Pietraszkiewicz, W., 1989. Geometrically nonlinear theories of thin elastic shells. *Adv. Mech.* 12, 51–130.
- Reddy, J.N., 2010. Nonlocal nonlinear formulations for bending of classical and shear deformation theories of beams and plates. *Int. J. Eng. Sci.* 48, 1507G–1518.
- Reissner, E., 1983. Linear and nonlinear theory of shells. *Thin Shell Structures*. Prentice Hall, New York, pp. 29–44.
- Roessle, A., Bishoff, M., Endland, W., Ramm, E., 1999. On the mathematical foundation of the (1,1,2)-plate model. *Int. J. Solids Struct.* 36, 2143–2168.
- Sansour, C., 1995. A theory and finite element formulation of shells at finite deformations involving thickness change: circumventing the use of a rotation tensor. *Arch. Appl. Mech.* 65, 194–216.
- Sansour, C., 1998. A unified concept of elastic-viscoplastic cosserat and micromorphic continua. *J. de Phys. IV Proc.* 8, 341–348.
- Sansour, C., Bednarczyk, H., 1995. The cosserat surface as shell model, theory and finite-element formulation. *Comput. Methods Appl. Mech. Eng.* 120, 1–32.
- Sansour, C., Bufler, H., 1992. An exact finite rotation shell theory, its mixed variational formulation, and its finite element implementation. *Int. J. Numer. Methods Eng.* 34, 73–115.
- Sansour, C., Kollmann, F.G., 1998. Large viscoplastic deformations of shells. Theory and finite element formulation. *Comput. Mech.* 21, 512–525.
- Sansour, C., Skatulla, S., 2009. A strain gradient generalised continuum approach for modelling elastic scale-effects. *Comput. Methods Appl. Mech. Eng.* 198, 1401–1412.
- Sansour, C., Skatulla, S., Hjjaj, M. Shell computations with higher gradients and scale effects, applications to stability problems. In press.
- Schieck, B., Pietraszkiewicz, W., Stumpf, H., 1992. Theory and numerical analysis of shells undergoing large elastic strains. *Int. J. Solids Struct.* 29, 689–709.
- Simo, J.C., Fox, D.D., Rifai, M.S., 1990. On a stress resultant geometrically exact shell model. Part III: Computational aspects of the nonlinear theory. *Comput. Methods Appl. Mech. Eng.* 79, 21–70.
- Skatulla, S., Sansour, C., 2008. Essential boundary conditions in meshfree methods via a modified variational principle. applications to shell computations. *Computer Assisted Mechanics and Engineering Sciences*.
- Sun, Yuzhou, Liew, K.M., 2008. Mesh-free simulation of single-walled carbon nanotubes using higher order cauchy-born rule. *Comput. Mater. Sci.* 42, 445–452.
- Wagner, G.J., Liu, W.K., 2000. Application of essential boundary conditions in mesh-free methods: a corrected collocation method. *Int. J. Numer. Methods Eng.* 47, 1367–1379.
- Wriggers, P., Gruttmann, F., 1993. Thin shells with finite rotations formulated in bigg stresses theory and finite-element formulation. *Int. J. Numer. Methods Eng.* 36, 2049G–2071.
- Zhilin, P.A., 1976. Mechanics of deformable directed surfaces. *Int. J. Solids Struct.* 12, 635–648.